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13. ABSTRACT (Maximum 200 words)

Specific aims:

The problems investigated in the project fall into three broad categories: (1) Modeling of twinning under high velocity impact (2) Constitutive equations for elasto-plastic response under large deformations with application to simple shear, and (3) variational approaches to the development of governing equations and boundary conditions for incorporating "lattice curvature effects" in plasticity with application to shear banding problems.

Results and their significance:

Using a novel "multiconfigurational" framework developed by us, we have developed models that account for deformation twinning under high velocity impact. The results show good agreement with experimental data. We found that the nonlinearity of the elastic response will lead to interesting softening behavior when the material undergoes simple shear deformations. We have developed a theory incorporating lattice curvature effects that can effectively simulate the formation of shear bands . We have also developed a new variational technique based on the maximization of the rate of energy dissipation that not only delivers the governing differential equations but also the accompanying boundary conditions. This work will allow for the development of computational codes that can delineate the relative influence of lattice curvature, twinning and strain softening on the formation of shear bands.

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Deformation twinning, lattice curvature, finite deformation plasticity

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Final Report

Foreword

Different dissipative processes such as twinning, solid to solid phase transitions, deformations of crystals due to slip, crystallization of polymers, scission and healing in multi-network polymers, flows of anisotropic liquids, growth and adaptation of biomaterials, etc., are usually described in terms of different theories . These studies fail to recognize that such dissipative processes, while different in important aspects, share many features in common. A central idea in common in all these processes is that during the process the natural configurations of the body in question, changes. Here, we use the general thermodynamic framework that was developed by us and that provides an unified way to look at these problems. This framework takes into account how the material stores energy, dissipates energy, produces entropy, etc., and gainfully exploits how the changes in the natural configurations are related to the rate of entropy production. This framework has been used to describe all the above dissipative processes quite faithfully. Here, we use this framework to study problems involving high velocity impact.

Problems involving high velocity impact of solids, involve regions of large plastic strains and plastic strain gradients being confined to a narrow region adjoining an inclusion, inhomogeneity or one of the boundaries of the domain of interest. One of the fundamental issues in the modeling of such localization is the identification of the parameters that quantify such concentrations. We have developed a theory incorporating lattice curvature effects that can effectively simulate the formation of shear bands . We have also developed a new variational technique based on the maximization of the rate of energy dissipation that not only delivers the governing differential equations but also the accompanying boundary conditions. This work will allow for the development of computational codes that can delineate the influence of coherent and incoherent interfaces on the formation of shear bands and hence help test the influence of the interface on the behavior of the material. We have also developed a Matlab based finite element program to solve a variety of boundary value problems for strain softening materials in order to study localization phenomena in a variety of circumstances.

Statement of the problem:

The problems investigated in the project fall into three broad categories: (1) Modeling of twinning under high velocity impact (2) Constitutive equations for elasto-plastic response under large deformations with application to simple shear, and (3) variational approaches to the development of governing equations and boundary conditions for incorporating "lattice curvature effects" in plasticity with application to shear banding problems.

Modeling of twinning under high velocity impact:

When materials such as Armco iron or depleted uranium are subject to impact, it is well known that two basic inelastic processes take place: slip and deformation twinning. Of these processes, slip has received quite a large amount of attention and several dislocation mechanics based criteria have been used for the modeling slip during impact. For example, Zerilli and Armstrong modeled the Taylor impact test using traditional plasticity theories and found significant discrepancies bewteen the theoretical predictions and experimental results. They attributed this to deformation twinning .

In a body that is undergoing twinning, there are many intermediate stress free configurations which correspond to thin layers of the parent and the twin juxtaposed in a ``fine" mixture, that is, these intermediate configurations can be viewed as a mixture of the stress-free configurations of the parent and the twin. Twinning can be induced due to temperature as well as applied tractions and usually proceeds gradually on a macroscale, though discrete conversions are possible. Recently, we used the fact that the body has more than one natural configuration and also distinct symmetries in these natural configurations to describe the process of twinning, taking into account the dissipation that accompanies twinning. Here, we shall discuss the configurational forces that come into play during the process of twinning. For our purposes, it suffices to introduce the bare essential features of the modeling.

Constitutive assumptions are made for the Helmholtz potential and the rate of dissipation. In order to better understand the twinning process, we studied the Taylor

impact test and , under the assumption that only twinning takes place, solved the dyamical equations using a finite element method.

Constitutive equations for elasto -plastic repsonse under large deformations

The aim of this work was fourfold (1) To develop a set of constitutive equations that are applicable to isotropic inelastic materials with large elastic and plastic strains using the multiconfigurational framework (Rajagopal and Srinivasa(1998a, 1998b)), in such a way as to generalize the central ideas (such as isotropy, constant elastic modulii, quadratic yield surfaces and non-hardening behavior) of the Prandtl-Reuss theory to finite deformations, (2) to examine the consequences of using a physically plausible criterion of maximum rate of mechanical dissipation, (3) to examine the relationship of the resulting models to the classical Prandtl-Reuss theory as well as other possible formulations (specifically those that rely on the use of a maximum plastic work postulate), and (4) to consider the effect of finite elastic strains on the response of the material subject to some simple homogenous deformations.

Lattice curvature effects in plasticity

We consider an elastic-plastic material whose strain energy depends not only on the elastic strain but also on its spatial gradient. The governing equations of motion are obtained by maximizing the rate of global energy dissipation. The resulting differential equations are specialized for the case where the strain energy depends also upon the lattice curvature, or the density of geometrically necessary dislocations.

Summary of important results

Twinning under high velocity impact

The results of the numerical calculations using the thermodyanamical approach developed by us show that twinning is confined to two regions – a large region near the impacted end of the specimen and a small region toward the rear. The latter region occurs due to the interaction between the incident and reflected waves. The extent of twinning and the energy absorbed show good agreement with experimental data on titanium in the regions where the twins dominate. Our results show that the energy absorbed during

twinning and the deformation due to twinning are relatively small, and the material twins more near the center line. We also demonstrate the dependence of the results on the initial grain size of the material. Specifically, by modeling two materials of widely differing grain sizes, we show that the large-grained material twins substantially more than the small-grained material.

Constitutive equations for elasto -plastic repsonse under large deformations

The use of a separate constitutive assumption for the rate of dissipation along with that for the Helmholtz potential together with the application of the maximum rate of dissipation criterion has been demonstrated here for the case of a finitely deforming elastic-plastic material.

It is shown that there are several different ways to generalize the classical Prandtl-Reuss equation while retaining their principal attributes namely, elastic isotropy, a quadratic yield function with no hardening and a normality rule. The present approach also contains the classical maximum plastic work criterion as a special case. Even for this special case, it is shown that choosing different plastic work conjugate variables is tantamount to choosing different forms for the rate of dissipation function.

An interesting observation is that, when one considers finite elastic deformations, although the material is nominally nonhardening, under conditions of simple shear, the shear stress versus shear strain graph has a negative slope beyond the yield point. This is due to the Poynting effect of finite elasticity and disappears for the case of small elastic but large total strains. Thus, data on the hardening behavior of such materials must take into account this effect in order to get meaningful models.

Lattice curvature effects in plasticity

One of the central difficulties with the addition of higher gradients of the plastic strain in traditional plasticity models has been the identification of physically meaningful additional boundary conditions. We address this question in two steps. First , rather than simply adding a strain gradient term to the yield function, we develop a thermodynamical framework for the inclusion of lattice curvature into the theory. Then, by using a global

maximization procedure that involves the use of an appropriately chosen dissipation function, we arrive at the governing equations as well as suitable, physically meaningful boundary conditions.

List of papers published under the ARO sponsorship

1. Baek, S., and Srinivasa, A. R., "A variational approach based on the maximization of the rate of dissipation in gradient plasticity", **Int. J. Nonlinear Mechanics** (accepted for publication).
2. Rajagopal, K. R., and Srinivasa, A. R., "On the role of the Eshelby energy-momentum tensor in materials with multiple natural configurations", **Mathematics and Mechanics of Solids,** (accepted for publication)
3. Mollica, F., Rajagopal , K. R., and Srinivasa A. R., "Inelastic behavior of materials subject to loading reversal", **Int. J. Plasticity,** 17 (8): 1119-1146, 2001.
4. Lapczyk, I., Rajagopal, K. R., and Srinivasa, A. R., "Twinning of a cylinder during the Taylor anvil test-Numerical calculations using a constitutive theory based on dual reference configurations", **Computer Methods in Applied Mechanics and Engineering,** 188, 527-541, 2000.
5. Lapcyzk, I., Rajagopal K. R., and Srinivasa, A. R., "Deformation during impact-numerical calculations using a constitutive theory based on multiple reference configurations", **Computer Methods in Applied Mechanics and Engineering**, 21, 20-27,1998
6. Srinivasa, A. R., "Finite deformations of a class of elastic plastic materials and the Poynting effect", **Int. J. Plasticity**, 17 (9): 1189-1214 , 2001.
7. Rengarajan, G., and Rajagopal, K. R., (2001), On the form for the Plastic Velocity Gradient $\mathbf{L}_p$ in Crystal Plasticity, **Journal of mathematics and mechanics of Solids**, 6, 471-480(2001)

Papers Presented in Meetings

1. Geometrically Necessary Dislocations and Localization Phenomena , 15th U. S. Army Symposium on Solid Mechanics, 12-24 April 1999, Myrtle Beach, South Carolina.

2. On Finite Plasticity and the Poynting Effect: ***SES Conference***, Columbia, SC, Oct 2000.
3. Two session organized on structural changes during impact: ***Society of Engineering Science***, Tempe, Arizona, Oct 19-23, 1996.
4. On a thermodynamical framework for dissipative processes: ***Army Research Labs,*** Aberdeen Proving Grounds, Aberdeen MD, March 25, 2002.

Scientific Personnel supported on this project

F. Mollica (Ph.D), S. Sivakumar (Research Scientist), S. Baek (working towards Ph. D).

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